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Search for pairs of scalar leptoquarks decaying into quarks and electrons or muons in $\sqrt{s} = 13$ TeV pp collisions with the ATLAS detector

The ATLAS Collaboration

A search for new-physics resonances decaying into a lepton and a jet performed by the ATLAS experiment is presented. Scalar leptoquarks pair-produced in pp collisions at $\sqrt{s} = 13$ TeV at the Large Hadron Collider are considered using an integrated luminosity of 139 fb^{-1}, corresponding to the full Run 2 dataset. They are searched for in events with two electrons or two muons and two or more jets, including jets identified as arising from the fragmentation of c- or b-quarks. The observed yield in each channel is consistent with the Standard Model background expectation. Leptoquarks with masses below 1.8 TeV and 1.7 TeV are excluded in the electron and muon channels, respectively, assuming a branching ratio into a charged lepton and a quark of 100%, with minimal dependence on the quark flavour. Upper limits on the aforementioned branching ratio are also given as a function of the leptoquark mass.

1 Introduction

Leptoquarks (LQs) are hypothetical colour-triplet particles that carry both baryon and lepton quantum numbers ($B \neq 0$, $L \neq 0$). As such, LQs couple simultaneously to both quarks and leptons, enabling direct transitions between the two. The spin of a LQ state is either 0 (scalar LQ) or 1 (vector LQ), and only the former is considered in this paper. Because of their SU(3) and SU(2) charge (colour and weak isospin, respectively), LQs can mediate flavour-changing neutral currents, and enable the violation of lepton flavour universality, which has been suggested as an explanation of recent measurements of B-meson decays [1–7]. New-physics models involving LQs might also resolve several interesting physical phenomena observed in nature. For instance, LQs can be used to explain the origins of the neutrino masses [8–11], as well as the origins of CP violation, thereby explaining the observed matter/antimatter asymmetry in the universe [12–14]. In addition, LQs could provide a satisfying connection between the apparent symmetry of lepton and quark generations, as well as unification of the electromagnetic and weak forces at high energy [15, 16].

At the LHC, the pair production of LQs is possible via gluon–gluon fusion and quark–antiquark annihilation, and the production cross-section largely depends only on the mass of the LQ, m_{LQ}. The cross-section is taken to be equivalent to that calculated [17–20] for the direct pair production of top squarks ($\tilde{t}$), the supersymmetric partners of the top quark, as both are massive, coloured, scalar particles with the same production modes.[1] Single production in association with a lepton is also possible, but the cross-section is model-dependent and it is not considered in this paper.

Diagrams depicting the lowest order possible production mechanisms that could enable scalar LQ pair production at the LHC are given in Figure 1, including strong and lepton t-channel exchange production [22].

LQs are assumed to couple to the quark–lepton pair via a single Yukawa interaction, with decays involving either charged leptons or neutrinos. The couplings are determined by two parameters, the model parameter β and the coupling parameter λ. The coupling to the charged lepton is given by $\sqrt{\beta}\lambda$ and the coupling to the neutrino by $\sqrt{1-\beta}\lambda$. Only the case of decays via electrons and muons is addressed in this paper. A traditional approach to LQ decay (such as in the Buchmüller–Rückl–Wyler model [23]), is to assume that LQs interact only with leptons and quarks of the same generation. This paper relaxes that restriction and considers cross-generational LQ decays. While the results are interpreted assuming one decay mode at a time (100% branching ratio, $\mathcal{B} = 1$), LQs with cross-generational decays might provide a possible solution to the anomalies in B-meson decays as observed by LHCb [24] if mixed decays into charged leptons (e.g. LQ $\rightarrow b\mu$ and $\rightarrow s\mu$) are allowed. Since the couplings to leptons and quarks are small ($\lambda \approx 1$), LQs have narrow decay widths (< 10% of m_{LQ}) and on-shell production dominates.

This paper presents a dedicated search for the pair production of LQs using the complete Run 2 dataset of 139 fb^{-1} of proton–proton (pp) collision data with $\sqrt{s} = 13$ TeV. Events are selected by requiring an oppositely charged electron or muon ($\ell = e, \mu$) pair and at least two jets that may be identified as originating from the fragmentation of c- or b-quarks (referred to as c-jets and b-jets, respectively) using dedicated tagging algorithms. The LQ decay channels that are searched for are therefore eq, μq, ec, μc, eb, and μb, where q is a u-, d- or s-quark. The results are presented as a function of m_{LQ}. This paper reports the first dedicated ATLAS search for cross-generational LQ decays using c- and b-jet identification.

[1] Recent calculations [21] show that diagrams involving t-channel lepton exchange might lead to corrections to the total cross-section at the percent level. Those are not taken into account for the interpretation of the results, but effects are expected to be within the uncertainties of the calculated cross-sections [17–20].

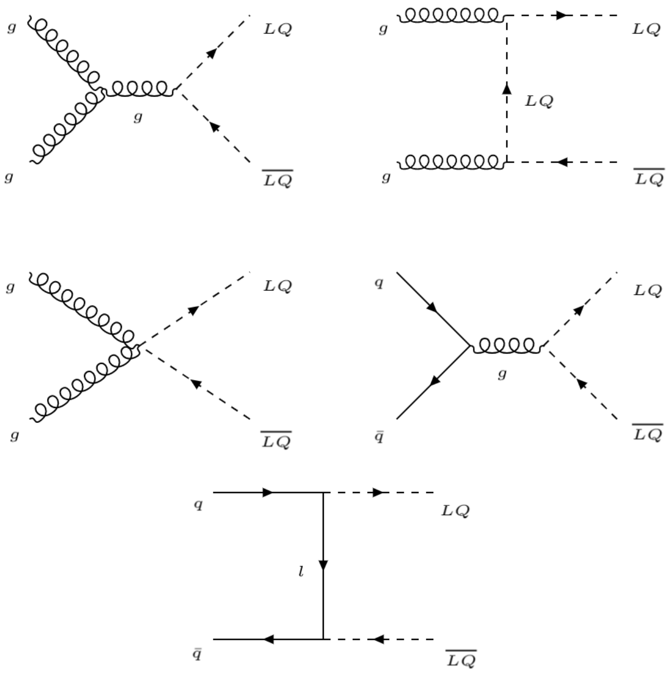

Figure 1: The primary mechanisms by which LQs can be pair produced at the LHC (gluon–gluon and quark–antiquark initiated) are shown.

The most recent searches for scalar leptoquark pairs from ATLAS and CMS were performed using 36.1 fb^{-1} of integrated luminosity at a 13 TeV centre-of-mass energy. A search by ATLAS for first- and second-generation LQs [25] did not use b-tagging in the signal regions and so excluded LQs decaying with 100% branching ratio ($\mathcal{B}$) into eQ or μQ, where $Q = u$, d, s, c or b, below a mass of 1400 GeV. CMS has also searched for first-generation [26] and second-generation [27] LQ pairs, excluding masses below 1435 GeV and 1530 GeV respectively for $\mathcal{B} = 1$. ATLAS has searched for third-generation up- and down-like LQ pairs, decaying into $t\nu/b\tau$ or $b\nu/t\tau$ [28] with limits on LQ masses up to 1100 GeV. CMS has excluded third-generation LQs decaying into τt [29] for $m_{\mathrm{LQ}} < 900$ GeV and τb [30] for $m_{\mathrm{LQ}} < 1020$ GeV, and cross-generational LQ decays into μt [31] for $m_{\mathrm{LQ}} < 1420$ GeV. Searches for new physics in ℓ+b-jets events have also been performed by ATLAS using 36.1 fb^{-1} of Run 2 data, targeting $B - L$ R-parity-violating supersymmetric models, and top squarks in particular [32]. As the production cross-section and decay modes of top squarks are equivalent to those of LQs, the exclusion limits on $m_{\tilde{t}}$ can be directly translated into m_{LQ} constraints. That search excludes top squarks with masses between 500 and 1200 GeV depending on the branching ratio into charged leptons and b-quarks.

2 The ATLAS detector

The ATLAS detector [33] is a multipurpose particle physics detector with a forward–backward symmetric cylindrical geometry and nearly 4π coverage in solid angle.[2] The inner tracking detector consists of silicon

[2] ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point in the centre of the detector. The positive x-axis is defined by the direction from the interaction point to the centre of the LHC ring, with the positive y-axis

pixel and microstrip detectors covering the pseudorapidity region $|\eta| < 2.5$, surrounded by a transition radiation tracker which enhances electron identification in the region $|\eta| < 2.0$. Between Run 1 and Run 2, a new inner pixel layer, the insertable B-layer [34, 35], was added at a mean sensor radius of 3.3 cm. The inner detector (ID) is surrounded by a thin superconducting solenoid providing an axial 2 T magnetic field, and by a fine-granularity lead/liquid-argon (LAr) electromagnetic calorimeter covering $|\eta| < 3.2$. A steel/scintillator-tile calorimeter provides hadronic coverage in the central pseudorapidity range ($|\eta| < 1.7$). The endcap and forward regions ($1.5 < |\eta| < 4.9$) of the hadronic calorimeter are made of LAr active layers with either copper or tungsten as the absorber material. An extensive muon spectrometer (MS) with an air-core toroidal magnet system surrounds the calorimeters. Three layers of high-precision tracking chambers provide coverage in the range $|\eta| < 2.7$, while dedicated fast chambers allow triggering in the region $|\eta| < 2.4$. The ATLAS trigger system consists of a hardware-based level-1 trigger followed by a software-based high-level trigger [36].

3 Data and Monte Carlo samples

The data analysed in this study correspond to 139 fb^{-1} of pp collision data collected by the ATLAS detector between 2015 and 2018 with a centre-of-mass energy of 13 TeV and a 25 ns proton bunch crossing interval. The uncertainty in the combined 2015–2018 integrated luminosity is 1.7% [37], obtained using the LUCID-2 detector [38] for the primary luminosity measurements. All detector subsystems were required to be operational during data taking and to fulfil data quality requirements. The average number of interactions in the same bunch crossing (pile-up) $\langle\mu\rangle$ was 33.7 for the combined dataset.

Candidate events were recorded by either single-muon or single-electron triggers [36] with various transverse momentum p_{T} (muons) or transverse energy E_{T} (electrons) thresholds. The lowest p_{T} (E_{T}) threshold without trigger prescaling was 24 (26) GeV and included a requirement on the energy in a cone around the lepton, referred to as 'isolation', that was not applied for triggers with higher thresholds. A trigger matching requirement [36] was applied, where the lepton must lie in the vicinity of the corresponding trigger-level object.

Dedicated Monte Carlo (MC) simulated samples are used to model SM processes and to estimate the expected signal yields. All samples were produced using the ATLAS simulation infrastructure [39] and GEANT4 [40]. A subset of samples use a faster simulation based on a parameterisation of the calorimeter response and GEANT4 for the other detector systems [39]. The simulated events are reconstructed with the same algorithms as used for data, and contain a realistic modelling of pile-up interactions. The pile-up profiles in the simulation match those of each dataset between 2015 and 2018, and are obtained by overlaying minimum-bias events, simulated using the soft QCD processes of PYTHIA 8 [41] using the NNPDF2.3LO set of PDFs [42] and a set of tuned parameters called the A3 tune [43].

Signal event samples with LQs pair produced via the strong interaction[3] were generated at next-to-leading order (NLO) with MADGRAPH5_aMC@NLO [44] v2.6.0 and interfaced to PYTHIA 8.230 for the modelling of parton showers (PS), hadronisation, and the underlying event with the A14 tune [45]. The matrix

pointing upwards, while the beam direction defines the z-axis. Cylindrical coordinates (r, ϕ) are used in the transverse plane, ϕ being the azimuthal angle around the z-axis. The component of momentum in the transverse plane is denoted by p_{T}. The pseudorapidity η is defined in terms of the polar angle θ by $\eta = -\ln\tan(\theta/2)$. Rapidity is defined as $y = 0.5\ln[(E+p_z)/(E-p_z)]$ where E denotes the energy, and p_z is the component of the momentum along the beam direction. The separation of two objects in η–ϕ space is given by $\Delta R = \sqrt{(\Delta\eta)^2 + (\Delta\phi)^2}$.

[3] It should be noted that t-channel lepton exchange production is not included in these samples.

Process		Generator	PDF set	PS and fragmentation/hadronisation	UE tune	Cross-section order
Top pair ($t\bar{t}$)		Powheg-Box v2 [49]	NNPDF 3.0 [50]	Pythia 8	A14	NNLO+NNLL [51]
Single-top	t-channel	Powheg-Box v1	NNPDF 3.0	Pythia 8	A14	NNLO+NNLL [52]
	s- and Wt-channel	Powheg-Box v2	NNPDF 3.0	Pythia 8	A14	NNLO+NNLL [53, 54]
W+jets, Z/Drell–Yan+jets		Sherpa 2.2.1 [55–59]	NNPDF 3.0	Sherpa	Default	NNLO [60]
Diboson		Sherpa 2.2.1 – 2.2.2	NNPDF 3.0	Sherpa	Default	NLO [55]

Table 1: List of generators used for the different background processes. Information is given about the underlying-event (UE) tunes, the PDF sets and the perturbative QCD highest-order accuracy (NLO, NNLO, and NNLL) used for the normalisation of the different samples.

element (ME) calculation was performed at tree level and includes the emission of up to two additional partons. The ME–PS matching was done using the CKKW-L [46] prescription, with a matching scale set to one quarter of the LQ mass. The NNPDF2.3 LO [42] parton distribution function (PDF) set was used. Samples with LQ mass set between 400 GeV and 2000 GeV were generated at mass intervals of 50 GeV within the range 800-1600 GeV, 100 GeV otherwise. Signal cross-sections are considered equivalent to those of pair-produced top squarks. They are calculated to approximate next-to-next-to-leading order (NNLO) in the strong coupling constant, adding the resummation of soft gluon emission at next-to-next-to-leading-logarithm (approximate NNLO+NNLL) accuracy [17–20]. The nominal cross-section and its uncertainty are derived using the PDF4LHC15_mc PDF set, following the recommendations of Ref. [47]. For LQ masses between 400 GeV and 2.0 TeV, the cross-sections range from 2.1 pb to 0.02 fb.

Background samples were simulated using different MC event generators depending on the process. All background processes are normalised to the best available theoretical calculation of their respective cross-sections. The event generators, the accuracy of theoretical cross-sections, the underlying-event parameter tunes, and the PDF sets used in simulating the SM background processes most relevant for this analysis are summarised in Table 1. For all samples, except those generated using Sherpa, the EvtGen v1.2.0 [48] program was used to simulate the properties of the b- and c-hadron decays.

4 Event reconstruction and object definitions

An event is selected if it passes at least one of the single-lepton trigger requirements described in the previous section. The event quality is checked to remove events with noise bursts or coherent noise in the calorimeters. At least one pp interaction vertex is required to be reconstructed in an event. The primary vertex is chosen to be the vertex with the highest summed p_{T}^2 of tracks with transverse momentum $p_{\mathrm{T}} > 0.5$ GeV which are associated with that vertex.

Electron candidates are reconstructed by matching inner-detector tracks to clusters of energy deposited in the EM calorimeter. Electrons must have $p_{\mathrm{T}}^e > 20$ GeV and $|\eta_e| < 2.47$. The associated track must have $|d_0|/\sigma_{d_0} < 3$ and $|z_0| \sin\theta < 0.5$ mm, where d_0 (z_0) is the transverse (longitudinal) impact parameter relative to the primary vertex and σ_{d_0} is the associated error in d_0. Candidates are identified with a likelihood method and must satisfy the 'medium' identification criteria according to Ref. [61]. The likelihood relies on the shape of the EM shower measured in the calorimeter, the quality of the track reconstruction, and the quality of the match between the track and the cluster. To suppress candidates originating from photon conversions, hadron decays, or jets misidentified as electrons, candidates are required to satisfy the gradient isolation criteria based on tracking and calorimeter measurements [61].

Muon candidates are reconstructed in the range $|\eta_\mu| < 2.5$ by combining tracks in the ID with tracks in the MS. For $2.5 < |\eta_\mu| < 2.7$, muons may be reconstructed solely from the MS track and a loose requirement on the compatibility of originating from the interaction point. An additional category of muons, called calorimeter-tagged muons, are used in the region $|\eta_\mu| < 0.1$, where the MS is only partially instrumented. For these muons the ID track must be compatible with energy deposits in the calorimeter consistent with a minimum-ionising particle.

All muon candidates must have $p_{\mathrm{T}}^{\mu} > 20$ GeV, $|d_0|/\sigma_{d_0} < 3$, and $|z_0|\sin\theta < 0.5$ mm. Muons from hadron decays are suppressed by imposing a track-based isolation requirement [62]. In order to improve the momentum resolution, further quality requirements are placed on the muons. The 'medium' quality requirements described in Ref. [62] are used for candidates with $p_{\mathrm{T}}^{\mu} < 800$ GeV. The main requirements are a minimum of three hits in the muon detector (except for $|\eta_\mu| < 0.1$, where there is a minimum of one hit) and for the difference between the momentum measurements in the ID and MS to have a q/p significance of less than 7.0. As muons with $p_{\mathrm{T}}^{\mu} > 800$ GeV have poorer momentum resolution, the more stringent 'high-p_{T}' quality requirements are imposed: muons with $|\eta_\mu| > 2.5$ without an inner-detector track are rejected; candidates must have hits in each of the three layers of the muon detector; and regions where the alignment is suboptimal are removed. The 'high p_{T}' quality requirements remove 20% of muons but improve the p_{T}^{μ} resolution by approximately 30% [62] above 1.5 TeV and suppress backgrounds.

Jets in the range $|\eta_j| < 4.5$ and $p_{\mathrm{T}}^{j} > 20$ GeV are reconstructed from energy deposits in the calorimeter [63], using the anti-k_t algorithm [64, 65] with a radius parameter of 0.4. To suppress jets arising from pile-up, a jet-vertex-tagging technique using a multivariate likelihood [66] is applied to jets with $p_{\mathrm{T}}^{j} \leq 60$ GeV, requiring that at least 60% of the total p_{T} of tracks in the jet be associated with the event's primary vertex.

To resolve the reconstruction ambiguities among electrons, muons, and jets, an overlap removal procedure is applied. First, any electron with the same ID track as a muon is rejected, unless it is a calorimeter-tagged muon, in which case the muon is removed. If the electron shares the same ID track with another electron, the one with lower p_{T} is discarded. Next, candidate jets with fewer than three associated tracks are discarded if they lie within a cone of $\Delta R = 0.2$ around a muon candidate, irrespective of the track requirement for the electron candidates. Subsequently, electrons within a cone of size $\Delta R = \min(0.4, 0.04 + 10\,\mathrm{GeV}/p_{\mathrm{T}})$ around a jet are removed. Last, muons within a cone, defined in the same way as for electrons, around any remaining jet are removed.

Jets in the range $|\eta_j| < 2.5$ are categorised as b-tagged or c-tagged jets, exploiting a multivariate algorithm that uses calorimeter and tracking information [67]. Jets are first tested using the b-tagging algorithm, which has an efficiency of about 70% for true b-jets with a rejection factor of about 8 for charm jets and about 300 for light-flavour jets [68]. In the $c\ell$ channels, jets that are not b-tagged are tested with the c-tagging algorithm, which has an efficiency of about 27% for true c-jets and approximate rejection factors of 12 for b-jets and 59 for light-flavour jets. The c-tagging algorithm is not used in the other channels.

When the selection requires two b-tagged jets, the substantial rejection rate of the tagging algorithm results in a significant statistical uncertainty for simulated Drell–Yan (DY) events containing only light-flavour jets or c-jets. Hence, instead of applying the b-tagging requirement, all events with c-jets or light-flavour jets are weighted by the probability that these jets pass it. This procedure, documented in Ref. [69], significantly increases the number of simulated events present after the full event selection, reducing the statistical uncertainty of the Drell–Yan background by up to a few orders of magnitude.

The event's missing transverse momentum (its modulus referred to $E_{\mathrm{T}}^{\mathrm{miss}}$) is computed as the negative vectorial sum of the transverse momenta of leptons and jets. The overlap between these is resolved according to Ref. [70, 71]. The $E_{\mathrm{T}}^{\mathrm{miss}}$ calculation also includes a track-based soft term [70] accounting for the contribution from particles from the primary vertex that are not already included in the $E_{\mathrm{T}}^{\mathrm{miss}}$ calculation.

5 Event selection

The event selection prioritises events consistent with scalar leptoquark production in high signal-to-background kinematic regions and has been optimised to reject signatures consistent with reducible backgrounds or poorly modelled event reconstruction.

Events are required to have exactly two electrons or two muons, oppositely charged and with transverse momenta greater than 27 GeV, ensuring the full efficiency of the trigger. At least two jets with $p_{\mathrm{T}}^{j} > 45$ GeV and $|\eta_j| < 2.5$ are required. Selections on the dilepton pair invariant mass, $m_{\ell\ell} > 130$ GeV, and transverse momentum, $p_{\mathrm{T}}^{\ell\ell} > 75$ GeV, are made to suppress background from the DY production and on-shell Z boson production. If there are more than two jets in the event, firstly those jets with tags are chosen as the candidate jets arising from the decays of the leptoquarks. For events with one tagged jet, the highest-p_{T} untagged jet is chosen as the second candidate. For events with zero tagged jets, the two highest-p_{T} jets are chosen. Events with more than two tagged jets are likely to be background and are rejected for the $c\ell$ and $b\ell$ channels. Background from $t\bar{t}$ production is suppressed by requiring $E_{\mathrm{T}}^{\mathrm{miss}}/\sqrt{H_{\mathrm{T}}} < 3.5\ \mathrm{GeV}^{1/2}$, where H_{T} is the scalar sum of the transverse momenta of all lepton candidates and selected jets in the event. This selection is preferable to a simple $E_{\mathrm{T}}^{\mathrm{miss}}$ selection as it is looser at higher p_{T} where the resolutions for the leptons and jets are worse.

Leptoquark candidates are identified from the two possible lepton–jet combinations by selecting the pairs closest in lepton–jet invariant mass, $m_{\ell j}$. SM background contributions are suppressed by requiring that

$$m^{\mathrm{asym}} = \frac{m_{\ell j}^{\mathrm{max}} - m_{\ell j}^{\mathrm{min}}}{m_{\ell j}^{\mathrm{max}} + m_{\ell j}^{\mathrm{min}}} < 0.4,$$

where $m_{\ell j}^{\mathrm{max}}$ and $m_{\ell j}^{\mathrm{min}}$ are the reconstructed masses of the two LQ candidates, ordered such that $m_{\ell j}^{\mathrm{max}} > m_{\ell j}^{\mathrm{min}}$. The selected region is further divided into a signal region (SR), requiring $m^{\mathrm{asym}} < 0.2$, and a sideband region (SB) where $0.2 < m^{\mathrm{asym}} < 0.4$. The SB is used in the maximum-likelihood fit, as described in Section 8, to help constrain the normalisation of the main backgrounds in a region with a low signal expectation. The results are presented as a function of the average of the two reconstructed leptoquark masses, $m_{\ell j}^{\mathrm{Av}} = (m_{\ell j}^{\mathrm{max}} + m_{\ell j}^{\mathrm{min}})/2$. The reconstructed mass resolution is found to not exceed 7% of the LQ mass in all channels.

A summary of the event selections for signal and SB regions is given in Table 2 before any specification of the flavour tags. The main selections for the Top control regions (CRs), used to aid in the estimation of the $t\bar{t}$ background and described in detail in Section 6, are also reported.

The SR and SB are further categorised to isolate kinematic regions that separate events consistent with light, charm and bottom quark production. These regions are defined by the b- and c-tagging results for the selected jets. An inclusive selection (referred to as pretag) is used for the $q\ell$ channels. Although the LQ $\to q\ell$ interpretations do not benefit from jet tagging when assuming that $\mathcal{B} = 1$ as considered in this paper, a selection of this kind might also provide sensitivity to cross-generational LQ decays if mixed decays into charged leptons are possible. The b-tagging selections are used in the $b\ell$ channels and target

<table>
<tr><th colspan="3">Preselection</th></tr>
<tr><td colspan="3">2 opposite charge leptons (e, μ)</td></tr>
<tr><td colspan="3">2 or more jets</td></tr>
<tr><td colspan="3">$p_{\mathrm{T}}^{e} > 27$ GeV, $|\eta_e| < 2.47$; $p_{\mathrm{T}}^{\mu} > 27$ GeV, $|\eta_\mu| < 2.7$</td></tr>
<tr><td colspan="3">$p_{\mathrm{T}}^{j} > 45$ GeV, $|\eta_j| < 2.5$</td></tr>
<tr><td colspan="3">$p_{\mathrm{T}}^{\ell\ell} > 75$ GeV</td></tr>
<tr><td colspan="3">$E_{\mathrm{T}}^{\mathrm{miss}}/\sqrt{H_{\mathrm{T}}} < 3.5$ GeV$^{1/2}$</td></tr>
<tr><td colspan="3">$m_{\ell\ell} > 130$ GeV</td></tr>
<tr><th>SB</th><th>SR</th><th>Top CR</th></tr>
<tr><td colspan="2">ee or $\mu\mu$</td><td>$e\mu$</td></tr>
<tr><td>$0.2 < m^{\mathrm{asym}} < 0.4$</td><td colspan="2">$m^{\mathrm{asym}} < 0.2$</td></tr>
</table>

Table 2: Summary of the preselection and region-specific selections applied before flavour tagging.

LQ $\to b\ell, \mathcal{B} = 1$ models, while both the b-tagging and c-tagging selections are used in the $c\ell$ channels, targeting LQ $\to c\ell, \mathcal{B} = 1$ models. In the $b\ell$ channels the events are split into those with zero, one, or two b-tags (referred to as 0-tag, 1-tag, and 2-tag, respectively). In the $c\ell$ channels the events are split into those with zero tags (untagged), at least one c-tag (c-tag), and at least one b-tag (b-tag). Events with one c-tagged jet and one b-tagged jet are placed in the c-tag category.

The signal and SB regions are not mutually exclusive between the search channels. The acceptance times detector efficiency for LQ events after all selections is highest in the electron channel qe for LQ masses around 1.3 TeV (62%) and between 45% and 55% for the mass range 400–2000 GeV in all channels. For muon-based selections, this is reduced to a maximum of 53% for LQ masses (around 900 GeV) in $q\mu$ channels and to about 30% for high LQ masses overall, due to the low efficiency of the high-p_{T} muon selection and the poorer efficiency of the $E_{\mathrm{T}}^{\mathrm{miss}}/\sqrt{H_{\mathrm{T}}}$ selection for muons than for electrons.

6 Background determination

The backgrounds in the analysis are estimated from simulated samples described in Section 3, with the aid of control and sideband regions for checks and estimates of systematic uncertainties. The dominant background in the pretag ($q\ell$), untagged ($c\ell$) and 0-tag ($b\ell$) SRs arises from DY production in association with two or more jets, followed by $t\bar{t}$ background. In the 1-tag, 2-tag, c-tag, and b-tag categories, the $t\bar{t}$ background dominates whilst DY background is subdominant. The DY background is further split into three categories, referred to as DY+light-jets, DY+c-jets, and DY+b-jets, based on the flavour of the heaviest quark as determined from simulation in either of the jets selected to reconstruct the LQ candidates.

To compensate for the limited number of events at high values of the average mass of the LQ candidates, a fit is made to the smoothly falling distributions for $t\bar{t}$ samples, and extrapolated to high $m_{\ell j}^{\mathrm{Av}}$ with the following function

$$f^{t\bar{t}}(m_{\ell j}^{\mathrm{Av}}) = a(m_{\ell j}^{\mathrm{Av}})^{b},$$

where a and b are the fitted parameters. In all cases, checks are performed to guarantee that the function reproduces the event yields at lower $m_{\ell j}^{\mathrm{Av}}$ values and that its cumulative distribution (starting from the highest $m_{\ell j}^{\mathrm{Av}}$ values) is consistent with the small integrated event yields available in the MC samples. Other SM processes, dibosons (WW, WZ, ZZ) and single-top production (mostly Wt), contribute less than 10%

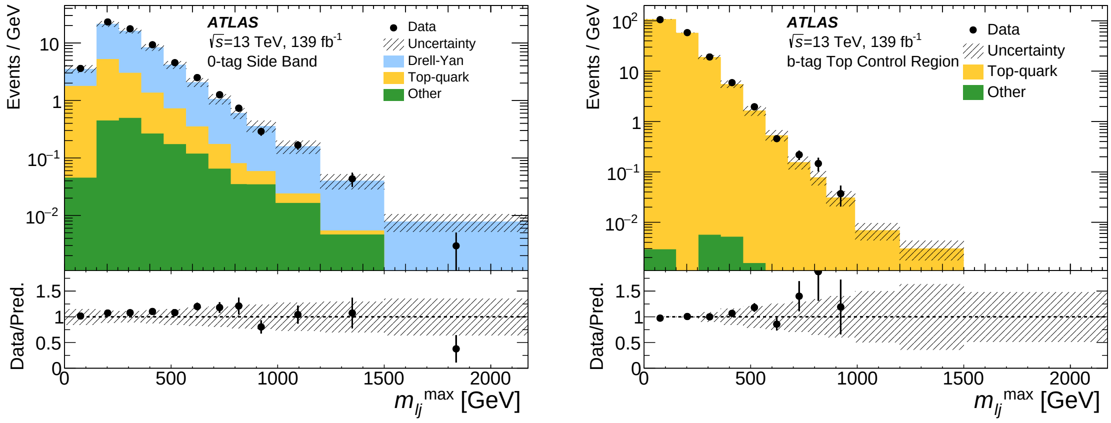

Figure 2: Distributions of $m_{\ell j}^{\max}$ in the combined be and $b\mu$ 0-tag SB for the $b\ell$ channels (left) and the b-tag Top CR for the $c\ell$ channels (right). The total modelling uncertainty combined with the MC statistical error is shown as the hatched band as explained in Section 7. The category 'Other' represents the sum of all SM background contributions except those from top-quark processes ($t\bar{t}$ and single-top) and, for the 0-tag SB distribution, Drell–Yan processes.

in all SRs and are estimated directly from MC samples. Rare processes such as $t\bar{t}V$, with $V = W, Z$ or Higgs bosons, and tribosons are negligible. Contributions from events where one or both electrons or muons are misidentified jets or non-promptly produced (referred to as 'fake' background) are checked using a same-sign lepton control region mirroring the SR selections. They are found to be dominated by single-electron fake contributions and well described by the $W(\rightarrow \ell\nu)$ + jets simulated samples, which are used for this estimate. A systematic error is assigned which covers any disagreement between the data and MC simulation in the same-sign region as described in Section 7.

The shape of the DY background is taken from simulation while the systematic uncertainty in the shape is determined by comparing data with the predictions in control regions dominated by the DY process as described in Section 7. The regions are an extended SB region which has $m^{\mathrm{asym}} > 0.4$ and a Z control region defined by inverting the selection on $m_{\ell\ell}$ (< 130 GeV) and removing the m^{asym} selection. The SB regions are used to validate the DY predictions.

An additional set of control regions is used to constrain the normalisation of the $t\bar{t}$ production background (Top CRs) in the pretag and tagged categories. The regions are identical to the default SR selections, corresponding to pretag for the $q\ell$ channels, c-tag and b-tag for the $c\ell$ channels, and 1-tag and 2-tag for the $b\ell$ channels, except that an electron–muon pair is taken in place of the same-flavour lepton pair. The 0-tag/untagged categories do not utilise this region as $t\bar{t}$ production is not dominant.

Figure 2 shows distributions of $m_{\ell j}^{\max}$ in the 0-tag SB region used to validate the DY predictions, and the b-tag Top CR for the $c\ell$ channels used for $t\bar{t}$ background contributions. Distributions are depicted before the profile-likelihood fit described below. Differences between data and MC predictions are used to estimate modelling uncertainties for these SM background processes, as explained in Section 7. The $m_{\ell j}^{\max}$ variable is used instead of $m_{\ell j}^{\mathrm{Av}}$ to retain more statistics in the tail of the distributions.

7 Systematic uncertainties

Several sources of experimental and theoretical systematic uncertainty in the signal and background estimates are considered.

For the LQ processes, experimental uncertainties in the signal yields are dominated by the uncertainty arising from lepton identification and jet energy scale and resolution ($q\ell$ channels) and from the b- and c-tagging efficiencies and mis-tagging rates ($c\ell$ and $b\ell$ channels). The uncertainties in the jet energy scale and resolution are based on their respective measurements in data [72, 73] and account for up to 2% of the signal yields. Uncertainties in electron identification efficiency, trigger efficiency, isolation efficiency, energy scale, and resolution amount to less than 6% [61, 62], while the muon uncertainties are less than 10% [61, 62]. The b- and c-tagging uncertainties are estimated by varying the η-, p_{T}- and flavour-dependent scale factors applied to each jet in the simulation within a range that reflects the systematic uncertainty in the measured tagging efficiency and mis-tag rates in data [67]. Uncertainties in b- and c-tagging are found to be less than 16% for the $c\ell$ channels and 19% for the $b\ell$ channels. The uncertainty due to the pile-up modelling [74] is typically less than 1%. Overall, the experimental uncertainties in the signals are between 1% and 20% of the yields, including the 1.7% uncertainty in the combined 2015–2018 integrated luminosity.

Theoretical uncertainties in the yields predicted using the approximate NNLO+NNLL cross-section are calculated for each LQ mass [17–20]. They are dominated by the uncertainties in the renormalisation and factorisation scales followed by the uncertainty in the PDFs, and range between 7% and 22% for LQ masses between 400 GeV and 2000 GeV. Additional uncertainties in the acceptance and efficiency in simulated signal samples are also taken into account. They are dominated by uncertainties due to the modelling of initial- and final-state radiation and renormalisation and factorisation scale variations in simulated signal samples and contribute up to 5% at LQ masses above 1 TeV.

Uncertainties in the modelling of the simulated SM background processes and in their theoretical cross-sections are also taken into account.

The shape uncertainty in the modelling of the DY background is defined by taking the largest difference between data and MC predictions in the control regions dominated by the DY process. The uncertainty is split into two parts, $\sigma^Z = \pm 0.2 \log(m_{\ell j}^{\mathrm{max}}/800\ \mathrm{GeV})$ and $\sigma^Z = \pm 0.4 \log(m_{\ell j}^{\mathrm{max}}/200\ \mathrm{GeV})$, to allow a shape difference between low and high $m_{\ell j}$. When added in quadrature these uncertainties approximately cover the observed disagreement. The $m_{\ell j}^{\mathrm{max}}$ variable is used instead of $m_{\ell j}^{\mathrm{Av}}$ as this leads to slightly larger, hence more conservative uncertainties. MC predictions were found to describe the data within these errors in the SB region. Since the DY shape modelling uncertainty is determined directly from the difference between the data and the simulation, most of the experimental uncertainties are not applied as this avoids double counting. Simulated samples also exhibit differences with respect to data, for example due to jet energy resolution, which might contribute to any disagreement. The b- and c-tagging uncertainties are, however, applied as these can change the normalisation between regions, and this is not taken into account in the modelling studies. The DY shape modelling uncertainty is treated as uncorrelated among DY+light-jets, DY+c-jets, and DY+b-jets processes. In addition to the shape uncertainties, the DY+c-jets and DY+b-jets processes are each assigned a 10% normalisation uncertainty, where this value represents the largest difference between data and MC simulation in the Z control region for any number of b-tags.

The $t\bar{t}$ modelling is determined in a similar way to the DY by comparing data and MC predictions in the Top control regions. Reasonable agreement between data and simulation is found and an error of $\sigma_{t\bar{t}} = \pm 0.5 \log(m_{\ell j}^{\mathrm{max}}/200\ \mathrm{GeV})$ is assigned to cover any possible differences. As in the DY estimates, the experimental uncertainties, with the exception of b- and c-tagging ones, are not applied to the $t\bar{t}$ simulation. The normalisation of the $t\bar{t}$ background is left as a free parameter in all fits.

The extrapolation uncertainty for the $t\bar{t}$ background is evaluated using a falling exponential function as an alternative to the functional form described in Section 6. Differences from the nominal form are as large as 100% at very high LQ candidate mass for all channels, but the impact on the results is minimal due to the low $t\bar{t}$ rate above 1.3 TeV.

Finally, normalisation uncertainties are associated with the predictions of diboson and single-top-quark processes, and non-prompt and misidentified leptons. A 30% uncertainty is assigned to the diboson predictions, dominated by theoretical modelling uncertainties and estimated as in Ref. [32]. The dominant uncertainty for single-top-quark predictions also arise from theoretical and modelling uncertainties of the Wt process. They are found to be around 35% and are computed using differences between the predictions from the nominal sample and those from additional samples differing in hard-scattering generator, modelling of the $t\bar{t}$ and Wt interference term, and other parameter settings. A 25% uncertainty is assigned to the background from non-prompt and misidentified leptons, computed using the difference between data and MC W+jets predictions in the same-sign leptons control sample described in Section 6.

8 Results

The data are compared with the expectation by performing maximum-likelihood fits to the distribution of $m_{\ell j}^{\mathrm{Av}}$ in the signal, sideband and Top control regions. The Top CRs contain a negligible signal expectation and are used to constrain the top-quark background. The SB regions are used to constrain the DY background. They have a low but non-negligible signal expectation and therefore are treated in the fit in the same way as the SRs. A separate fit is performed for each signal hypothesis. Confidence intervals are based on a profile-likelihood-ratio test statistic [75], assuming asymptotic distributions for the test statistic.[4] The systematic uncertainties affecting the signal and background normalisations and shapes across categories are parameterised by making the likelihood function depend on dedicated nuisance parameters, constrained by additional Gaussian or log-normal probability terms.

For the $q\ell$ signals, the pretag SR, SB, and Top CR are used. For the $c\ell$ channels, the SR and SB in untagged, c-tag and b-tag categories are used together with the Top CR for c-tag and b-tag. For the $b\ell$ channels, the SR and SB in 0-, 1-, and 2-tag categories are used together with the Top CR in 1- and 2-tag. In all fits the DY and $t\bar{t}$ normalisations are treated as a single free parameter while different uncertainties in the shapes of distributions are assigned to the events as described in Section 7.

All other backgrounds are set to their MC expectations and are allowed to float within their respective uncertainties.

The event yields in the SR for all channels are listed in Tables 3 to 5. The SM background expectations resulting from the fits are reported showing statistical plus systematic uncertainties. The largest background contribution in $q\ell$ channels arises from DY+ light-jets, whilst the contribution from $t\bar{t}$ is largest for the signal regions relevant for the $c\ell$- and $b\ell$-jet channels. Single-top-quark and diboson processes as well as misidentified/non-prompt lepton contributions are subdominant in all regions. No significant differences

[4] Cross-checks with sampling distributions generated using pseudo-experiments were performed to test the accuracy of the asymptotic approximation for the high-mass part of the lepton–jet spectrum. The approximation is found to lead to limits that are slightly stronger than those obtained with pseudo-experiments, i.e. about 15% at 1.8 TeV, independent of the channel. The impact of this approximation on the mass limits is below 50 GeV.

are observed between expected and observed yields in all selections and channels considered. Since the SRs are not mutually exclusive, the same data are used across the various channels.

Figures 3 to 7 show comparisons between the observed data and the post-fit SM predictions for $m_{\ell j}^{\mathrm{Av}}$ for all signal regions in the $q\ell$, $c\ell$, and $b\ell$ channels. In each case, the expected distribution for one scenario with LQ mass of 1 TeV is shown for illustrative purposes, considering LQ $\rightarrow qe/q\mu$ for the pretag channels (with $q = u$-, d- or s-quark), LQ $\rightarrow ce/c\mu$ for the $c\ell$ channels, and LQ $\rightarrow be/b\mu$ for the $b\ell$ channels.

As no evidence of an excess at any mass in any of the channels was found, upper limits on the leptoquark production cross-section are computed at the 95% confidence level using a modified frequentist $\mathrm{CL_s}$ method [75, 76]. The limits are shown in Figure 8 as a function of m_{LQ} for a 100% branching ratio into charged leptons. They were calculated for LQ masses of the generated samples, and a linear interpolation has been made between mass points. The theoretical prediction for the cross-section of scalar leptoquark pair production is shown by the solid line along with the uncertainties. Exclusion limits are driven by the small number of data events populating the high-mass part of the lepton–jet spectrum. The limits at large m_{LQ} are more stringent for decays with electrons than for decays with muons, due to the better electron resolution at high p_{T}. The decays involving c- and b-quarks have slightly lower cross-section limits over most of the mass range, due to the lower rate of SM background contributions in the tagged categories.

The results of the fit may also be expressed as limits on the branching ratio into charged leptons as shown in Figure 9. In this case, it is assumed that there is zero acceptance for LQ decays involving neutrinos or top quarks. Furthermore, it is assumed that the LQs can decay into only one specific combination of lepton flavour and quark flavour. The $\mathcal{B}$ limit is computed as $\sqrt{\sigma_{\mathrm{obs}}/\sigma_{\mathrm{theory}}}$, where σ_{obs} is the observed LQ pair production cross-section exclusion limit with $\mathcal{B} = 1$ into charged leptons and σ_{theory} is the theoretical cross-section. Constraints on the LQ masses are reduced by no more than 20% for $\mathcal{B} = 0.5$, and LQs with mass around 800 GeV can be excluded for branching ratios into charged leptons as low as 0.1 (up to 900 GeV for $b\ell$ channels). This result improves upon the sensitivity of previous scalar LQ searches by about 300–400 GeV in LQ mass depending on the lepton flavour, and it establishes for the first time limits on cross-generational LQ decays using dedicated c- and b-tagging algorithms.

	LQ → qe	LQ → $q\mu$
$t\bar{t}$	1790 ± 220	1910 ± 240
Single top	390 ± 110	430 ± 120
DY+light-jets	2820 ± 180	3040 ± 180
DY+c-jets	521 ± 93	528 ± 90
DY+b-jets	233 ± 44	252 ± 46
W+jets	126 ± 32	8.5 ± 2.2
Diboson	31.8 ± 9.6	12.4 ± 3.7
Fitted SM background events	5910 ± 67	6185 ± 77
Observed events	5881	6169
Signal (m_{LQ} = 1 TeV)	591 ± 45	503 ± 27
Signal (m_{LQ} = 1.5 TeV)	22.1 ± 1.7	15.4 ± 1.0

Table 3: Observed and expected numbers of events in pretag SRs for LQ → $q\ell$, where SM predictions are the result of fits performed using 139 fb^{-1} of data. The uncertainties quoted for the fitted SM background include both the statistical and systematic components. Yields for two LQ scenarios are also shown for comparison.

		LQ → ce			LQ → $c\mu$	
	untagged	b-tag	c-tag	untagged	b-tag	c-tag
$t\bar{t}$	291 ± 18	964 ± 51	227 ± 14	293 ± 16	1049 ± 50	237 ± 14
Single top	35 ± 11	129 ± 39	28.7 ± 9.0	37 ± 10	166 ± 46	38 ± 11
DY+light-jets	2872 ± 74	32.3 ± 8.6	101 ± 11	3120 ± 71	29.0 ± 9.4	123 ± 13
DY+c-jets	367 ± 49	80 ± 12	135 ± 17	340 ± 46	67 ± 10	155 ± 20
DY+b-jets	39.4 ± 5.7	166 ± 24	31.5 ± 4.8	40.4 ± 5.7	165 ± 23	35.1 ± 5.2
W+jets	101 ± 26	10.2 ± 2.7	7.5 ± 2.0	6.3 ± 1.6	1.39 ± 0.36	0.81 ± 0.21
Diboson	23.5 ± 7.2	2.58 ± 0.79	3.6 ± 1.1	9.0 ± 2.7	1.21 ± 0.37	1.45 ± 0.44
Fitted SM events	3728 ± 53	1384 ± 26	534 ± 17	3846 ± 55	1478 ± 26	591 ± 18
Observed events	3714	1366	535	3824	1484	591
Signal (m_{LQ} = 1 TeV)	312 ± 26	71 ± 12	129 ± 13	265 ± 17	58.0 ± 9.1	111.5 ± 9.5
Signal (m_{LQ} = 1.5 TeV)	13.7 ± 1.2	2.33 ± 0.38	3.10 ± 0.30	9.72 ± 0.69	1.49 ± 0.28	1.99 ± 0.20

Table 4: Observed and expected numbers of events in untagged, c- and b-tag SRs for LQ → $c\ell$, where SM predictions are the result of fits performed using 139 fb^{-1} of data. The uncertainties quoted for the fitted SM background include both the statistical and systematic components. Yields for two LQ scenarios are also shown for comparison.

		LQ → be			LQ → $b\mu$	
	0-tag	1-tag	2-tag	0-tag	1-tag	2-tag
$t\bar{t}$	469 ± 22	919 ± 33	255 ± 11	487 ± 22	1001 ± 35	295 ± 12
Single top	51 ± 11	109 ± 24	48 ± 10	48 ± 10	122 ± 25	49 ± 10
DY+light-jets	3035 ± 95	29.2 ± 8.0	0.105 ± 0.057	3318 ± 93	36 ± 11	0.099 ± 0.059
DY+c-jets	479 ± 77	92 ± 15	1.68 ± 0.34	464 ± 75	75 ± 13	1.61 ± 0.33
DY+b-jets	54.2 ± 7.7	165 ± 23	25.9 ± 3.6	52.5 ± 7.6	151 ± 22	21.1 ± 3.0
W+jets	113 ± 29	9.4 ± 2.4	1.02 ± 0.27	7.5 ± 1.9	0.97 ± 0.25	0.110 ± 0.028
Diboson	27.8 ± 8.5	2.63 ± 0.81	0.33 ± 0.10	10.8 ± 3.2	1.21 ± 0.37	0.141 ± 0.043
Fitted SM events	4229 ± 57	1326 ± 25	332.4 ± 9.0	4389 ± 59	1387 ± 25	367.1 ± 9.3
Observed events	4214	1314	316	4367	1408	340
Signal (m_{LQ} = 1 TeV)	102 ± 13	237 ± 19	149 ± 13	87 ± 11	200 ± 12	124.1 ± 8.7
Signal (m_{LQ} = 1.5 TeV)	5.69 ± 0.90	8.72 ± 0.76	3.57 ± 0.33	3.89 ± 0.61	6.11 ± 0.50	2.38 ± 0.20

Table 5: Observed and expected numbers of events in 0-, 1- and 2-tag SRs for LQ → $b\ell$, where SM predictions are the result of fits performed using 139 fb^{-1} of data. The uncertainties quoted for the fitted SM background include both the statistical and systematic components. Yields for two LQ scenarios are also shown for comparison.

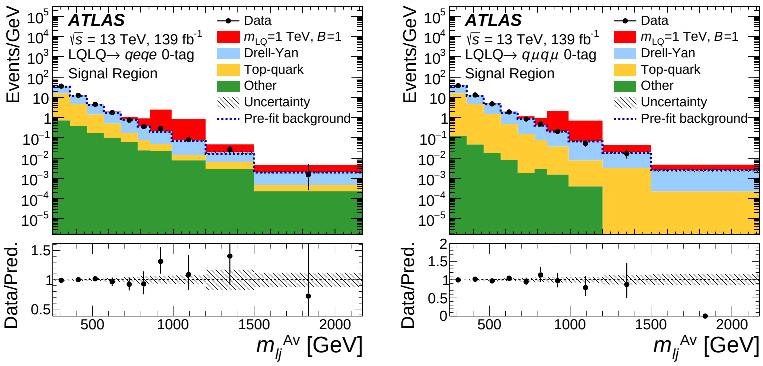

Figure 3: Post-fit distributions of $m_{\ell j}^{\mathrm{Av}}$ in the pretag signal regions for the qe (left) and $q\mu$ (right) channels. The expected signals, shown for $m_{\mathrm{LQ}} = 1$ TeV and $\mathcal{B}(\mathrm{LQ} \to qe/q\mu) = 1$, are shown for illustrative purposes. The category 'Top quark' refers to $t\bar{t}$ and single-top-quark processes. The category 'Other' refers to diboson and W+jet production. The hatched band represents the total uncertainty in the background predictions. Data and predictions outside the depicted mass range are not used in the fit and not shown.

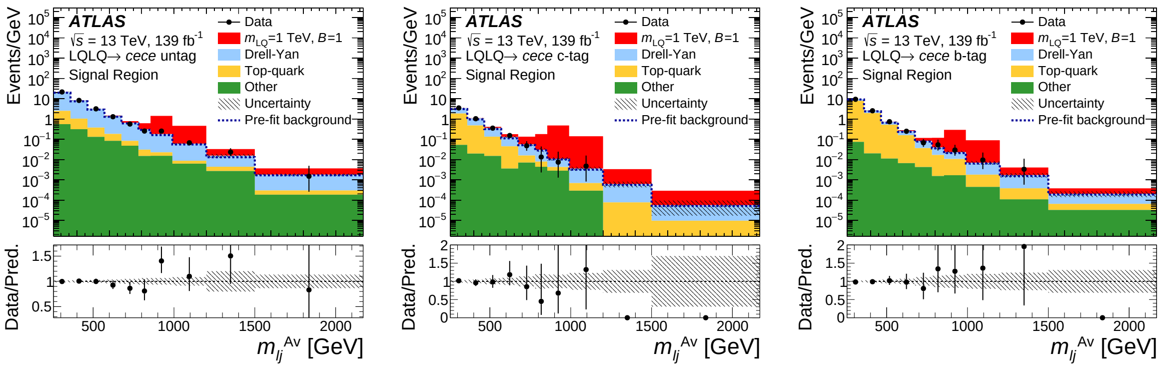

Figure 4: Post-fit distributions of $m_{\ell j}^{\mathrm{Av}}$ in the ce signal regions: untagged (left), c-tag (middle), and b-tag (right). The expected signals, shown for $m_{\mathrm{LQ}} = 1$ TeV and $\mathcal{B}(\mathrm{LQ} \to ce) = 1$, are shown for illustrative purposes. The category 'Top quark' refers to $t\bar{t}$ and single-top-quark processes. The category 'Other' refers to diboson and W+jet production. The hatched band represents the total uncertainty in the background predictions. Data and predictions outside the depicted mass range are not used in the fit and not shown.

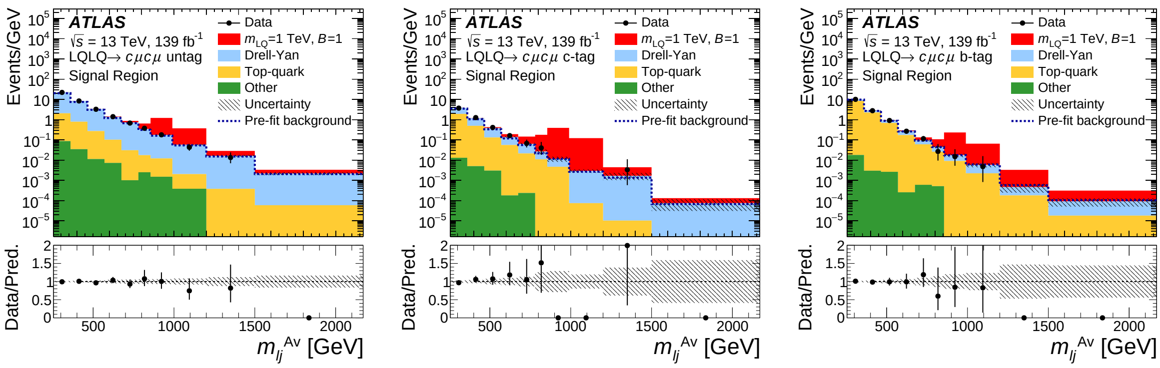

Figure 5: Post-fit distributions of $m_{\ell j}^{\mathrm{Av}}$ in the $c\mu$ signal regions: untagged (left), c-tag (middle), and b-tag (right). The expected signals, shown for $m_{\mathrm{LQ}} = 1$ TeV and $\mathcal{B}(\mathrm{LQ} \to c\mu) = 1$, are shown for illustrative purposes. The category 'Top quark' refers to $t\bar{t}$ and single-top-quark processes. The category 'Other' refers to diboson and W+jet production. The hatched band represents the total uncertainty in the background predictions. Data and predictions outside the depicted mass range are not used in the fit and not shown.

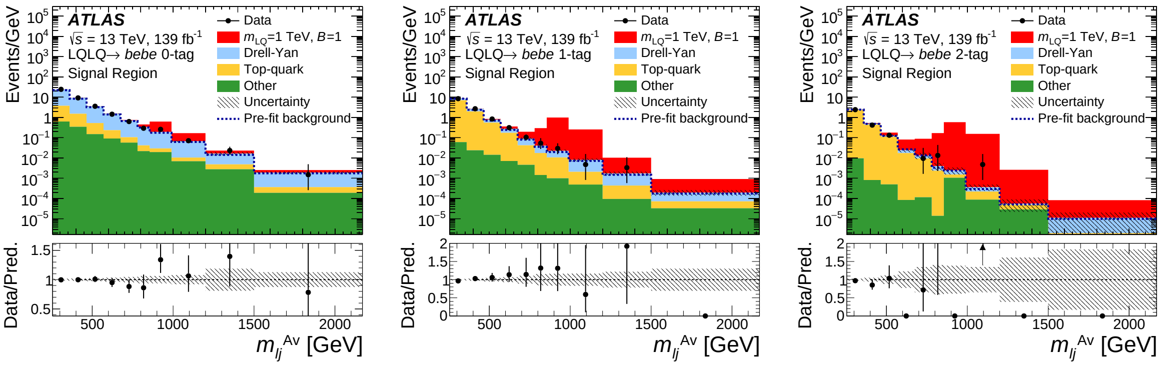

Figure 6: Post-fit distributions of $m_{\ell j}^{\mathrm{Av}}$ in the *be* signal regions: 0-tag (left), 1-tag (middle), and 2-tag (right). The expected signals, shown for $m_{\mathrm{LQ}} = 1$ TeV and $\mathcal{B}(\mathrm{LQ} \rightarrow be) = 1$, are shown for illustrative purposes. The category 'Top quark' refers to $t\bar{t}$ and single-top-quark processes. The category 'Other' refers to diboson and W+jet production. The hatched band represents the total uncertainty in the background predictions. Data and predictions outside the depicted mass range are not used in the fit and not shown.

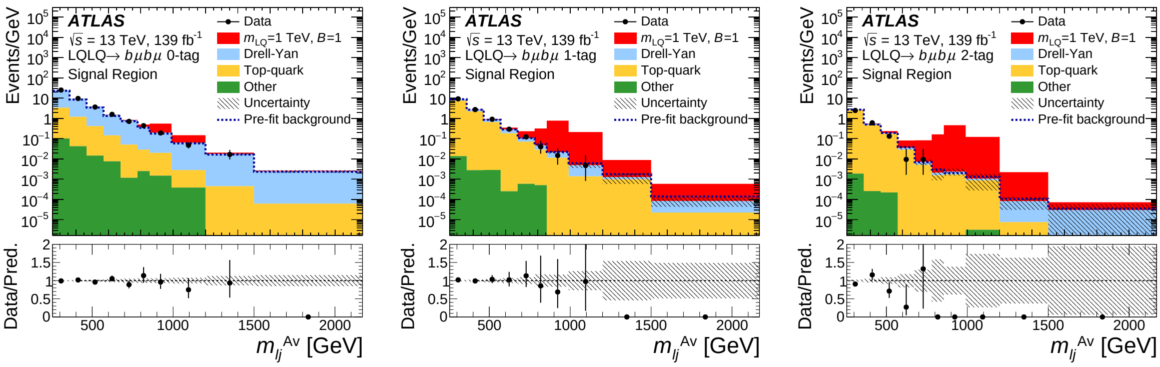

Figure 7: Post-fit distributions of $m_{\ell j}^{\mathrm{Av}}$ in the $b\mu$ signal regions: 0-tag (left), 1-tag (middle), and 2-tag (right). The expected signals, shown for $m_{\mathrm{LQ}} = 1$ TeV and $\mathcal{B}(\mathrm{LQ} \rightarrow b\mu) = 1$, are shown for illustrative purposes. The category 'Top quark' refers to $t\bar{t}$ and single-top-quark processes. The category 'Other' refers to diboson and W+jet production. The hatched band represents the total uncertainty in the background predictions. Data and predictions outside the depicted mass range are not used in the fit and not shown.

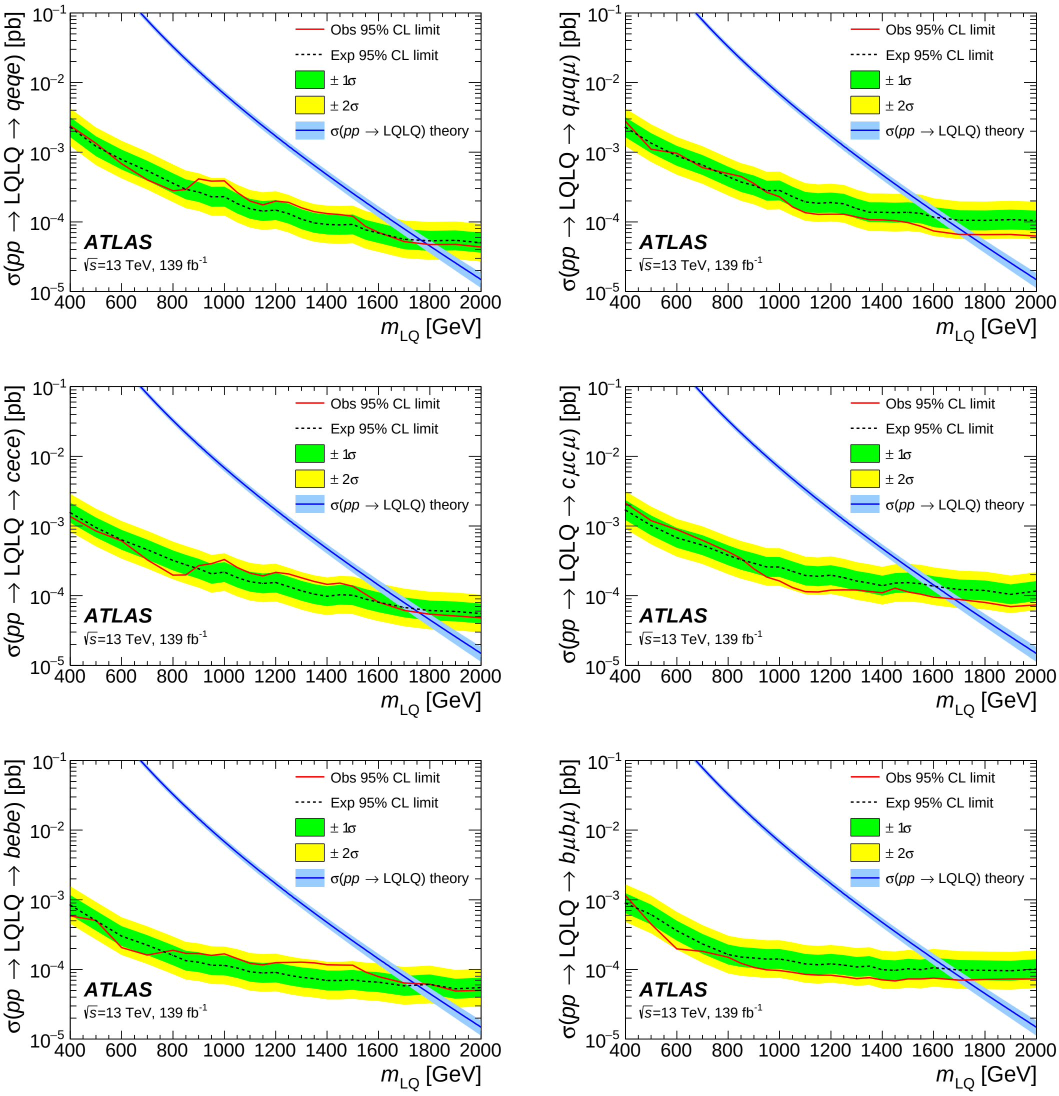

Figure 8: The observed and expected limits on the leptoquark pair production cross-section at 95% CL for $\mathcal{B} = 1$ into electrons or muons, shown as a function of m_{LQ} for the different leptoquark channels. The green and yellow bands show the $\pm1\sigma$ and $\pm2\sigma$ ranges of the expected limit. Also included on the plots is the expected theoretical cross-section. The thickness of the theory curve represents the theoretical uncertainty from PDFs, renormalisation and factorisation scales, and the strong coupling constant α_{S}.

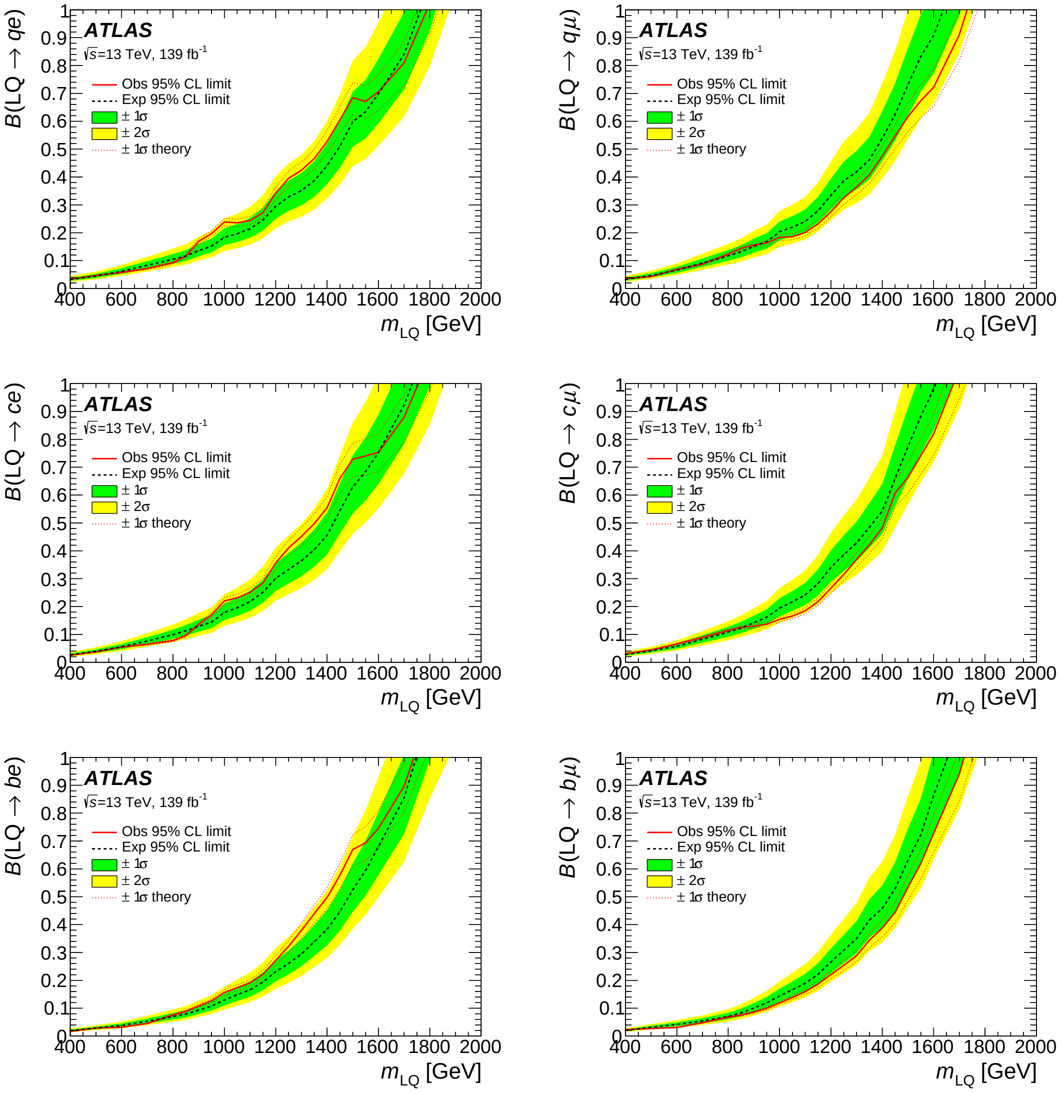

Figure 9: The observed and expected limits on the leptoquark branching ratio $\mathcal{B}$ into a quark and an electron or a muon at 95% CL, shown as a function of m_{LQ} for the different leptoquark channels. The green and yellow bands show the $\pm 1\sigma$ and $\pm 2\sigma$ ranges of the expected limit. The error band on the observed curve represents the uncertainty in the theoretical cross-section from PDFs, renormalisation and factorisation scales, and the strong coupling constant α_{S}.

9 Conclusion

A search for a new-physics resonances decaying into a lepton and a jet performed by the ATLAS experiment is presented. Scalar leptoquarks, pair produced in pp collisions at $\sqrt{s} = 13$ TeV at the LHC, are considered using an integrated luminosity of 139 fb^{-1}, corresponding to the full Run 2 dataset. Leptoquarks are searched for in events with two electrons or muons and two or more jets. Tagging algorithms are used to identify jets arising from the fragmentation of b-quarks (b-jets) and, for the first time, of c-quarks (c-jets). The observed yield in each channel is consistent with SM background expectations. Leptoquarks with masses below 1.8 TeV and 1.7 TeV are excluded in the electron and muon channels, respectively, assuming a branching ratio into a charged lepton and a quark of 100%, with minimal dependency on the quark flavour. Upper limits on the aforementioned branching ratio are also presented. LQs with masses up to around 800 GeV can be excluded for branching ratios into charged leptons as low as 0.1, assuming that there is zero acceptance for LQ decays involving neutrinos or top quarks, and that only one charged lepton plus quark decay mode at the time is possible. This result improves upon the sensitivity of previous scalar LQ searches by about 300–400 GeV in LQ mass depending on the lepton flavour, and it establishes for the first time limits on cross-generational LQ decays using dedicated c- and b-jet identification algorithms.

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